



DOCTORAL DISSERTATION

**ATOMIC SPECTROSCOPY WITH ION ACCELERATORS
AND
LASER – PRODUCED PLASMAS**

BY

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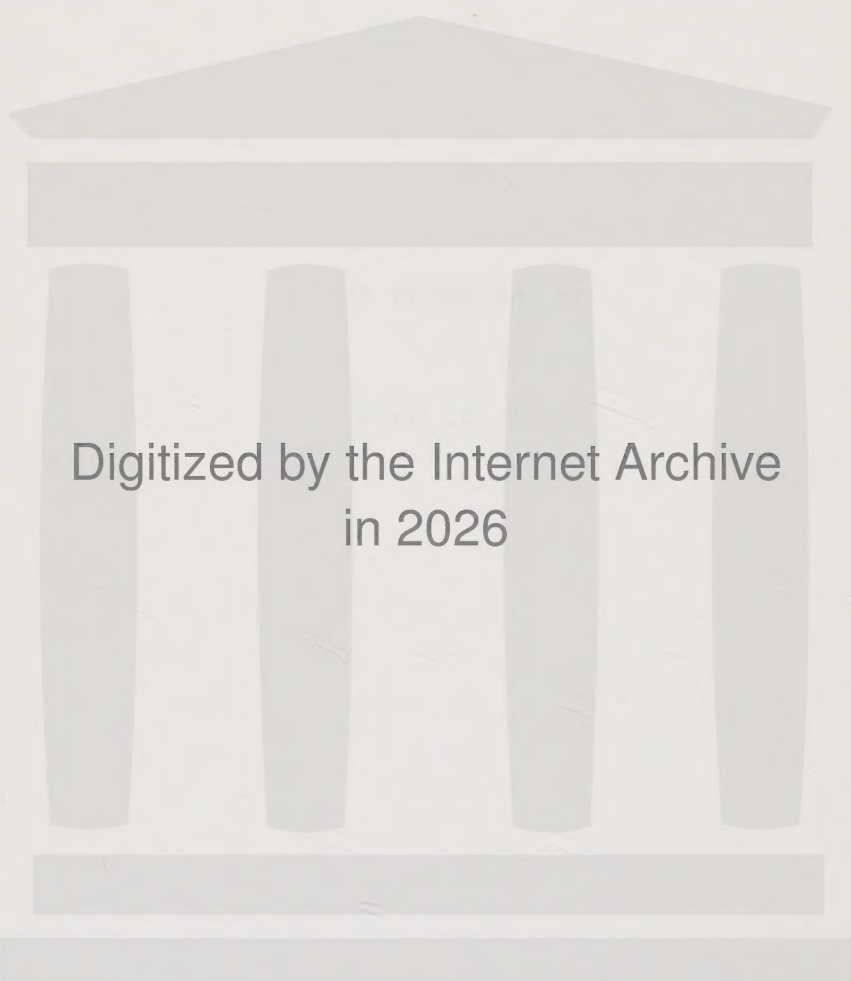
DOCTORAL DISSERTATION

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1. INTRODUCTION

Atomic spectroscopy is one of the oldest fields in modern physics. Already in the last century, physicists were using empirical methods [1] to explain the origin of spectral lines. In the beginning of this century Bohr introduced quantum theory to the study of the hydrogen atom. Quantum theory was later developed into Quantum mechanics by Schrödinger and others. One of the approximations to the Schrödinger equation, the Hartree-Fock equations, proved to be a powerful tool in the analysis of atomic spectra. At the same time, experimental methods were developing along with the advancement of optics and the arrival of new light sources.

In this thesis we have used two very different light sources: foil-excited fast ions from an accelerator and laser-produced plasmas. Using the first method we have studied spectra, lifetimes from decay curves and excitation mechanisms. The other source permitted us to study spectra at high resolution.

We have obtained information on energy levels, transition arrays and lifetimes in highly ionised atoms. Such information is important for the understanding of atomic structure, and is also applicable in astrophysics and plasma physics. The study of astronomical objects such as the sun, stars and interstellar space, benefits from knowledge of atomic data [2]. Another important application of atomic spectroscopy is in the study of various processes observed in high temperature plasmas such as Tokamaks, Theta-pinch, etc. Qualitative and quantitative investigations of the plasma impurities are facilitated

and information can also be obtained concerning the plasma temperature, electron density and plasma turbulence [3-10].

2. LIST OF PUBLICATIONS AND COMMENTS ON THE PAPERS

This thesis consists of 6 published papers and 2 papers accepted for publication. They are divided into 4 groups: 1 - The analysis of spectra with the beam-foil method; 2 - Lifetime measurements with the beam-foil method; 3 - Excitation mechanisms with molecular beams; 4 - Analyses of spectra from laser-produced plasmas.

GROUP 1. ANALYSES OF SPECTRA WITH THE BEAM-FOIL METHOD

Paper 1. Beam-foil study of $2p^43s$, $3p$ and $3d$ configurations in S VIII.

A. Trigueiros and C. Jupén.

Accepted for publication in Nuclear Instruments and Methods:B (Proceedings of the International Conference of Highly Ionised Atoms, Oxford - England, July 1984).

In this paper the spectrum of seven times ionised sulphur, S VIII, has been observed from 450 to 1150 Å. Thirty lines have been identified as combinations between levels of the $2p^43s$, $3p$ and $3d$ configurations. The term of the ground con-



figuration is an inverted 2P and thus only levels of the $2p^43s$ and $2p^43d$ configurations with $J \leq 5/2$ can combine with the ground term. In this analysis all levels with $J > 5/2$ that previously were unknown are established. For the $2p^43p$ configuration all but $(^3P)^2P_{3/2}$, $(^3P)^2P_{1/2}$, $(^1S)^2P_{3/2}$ and $(^1S)^2P_{1/2}$ levels were identified.

Paper 2. Analysis of the $2p^43s$, $3p$ and $3d$ configurations in seven times ionised sulphur (S VIII).

A. Trigueiros and C. Jupén

Accepted for publication in *Physica Scripta*.

This is a extension of paper 1, but here we have identified about 40 lines. Their identification is supported by isoelectronic comparisons along the F I sequence and parametric calculations. The values of the fitted parameters are given and a comparison is made with the Hartree-Fock parameters.

Paper 3. Transitions in Multiply Excited F VI and F VII.

I. Martinson, B. Denne, J.O. Ekberg, L. Engström, S. Huldt, C. Jupén, U. Litzén, S. Mannervik and A. Trigueiros.

Physica Scripta 27, 201 (1983).

In this paper we have identified the transitions $1s2s2p^2\ ^5P-1s2p^3\ ^5S$ in Be-like F VI and $1s2s2p\ ^4P-1s2p^2\ ^4P$ in Li-like

F VII. The beam-foil method is very efficient in populating such inner-shell excited configurations. The fine structure separations were determined in both ions and the results serve as experimental tests of accurate theoretical calculations, e.g. those based on the multiconfiguration Dirac-Fock (MCDF) method.

GROUP 2. LIFETIME MEASUREMENTS WITH THE BEAM-FOIL METHOD

Paper 4. Lifetimes of the $2s2p\ ^1P$ level in Be-like N IV and O V Obtained from Beam-foil Experiments and Extensive Cascade Analyses.

L. Engström, B. Denne, J.O. Ekberg, K.W. Jones, C. Jupén, U. Litzen, Weng Tai Meng, A. Trigueiros and I. Martinson. *Physica Scripta* 24, 551 (1981).

Paper 5. Accurate Experimental Lifetimes of Excited Levels in Sodium like Sulphur, S VI.

J.O. Ekberg, L. Engström, S. Bashkin, S. Huldt, S. Johansson, C. Jupén, U. Litzen, A. Trigueiros and I. Martinson. *Physica Scripta* 27, 425-430 (1983).

Paper 6. Lifetimes of the $^2P_{1/2}$, $^2P_{3/2}$ and $^2D_{3/2}$, $^2D_{5/2}$ Levels in Cl VII.

C. Jupén, L. Engström, S. Huldt, A. Trigueiros, J.O. Ekberg,
U. Litzen and I. Martinson.

Physica Scripta 29, 226-229 (1984).

The lifetimes and oscillator strengths in the Be I and Na I isoelectronic sequences have been studied by several investigators. A comparison between the experimental f -values for the resonance lines, obtained by the beam-foil method, and the results of accurate theoretical calculations often shows systematic disagreements. It has been suggested that the reason for this is incomplete correction for cascades in the analyses of the beam-foil decay curves. In our experiments the cascading transitions were measured and the data analysed using the ANDC technique of Curtis [46]. The results are in good agreement with theoretical values.

GROUP 3. EXCITATION MECHANISMS WITH MOLECULAR IONS

Paper 7. Dissociation of CN^+ into Atomic Excited States after Acceleration in a Tandem Accelerator.

H.G. Berry, L. Engström, R. Hellborg, S. Huldt, C. Jupén, A. Trigueiros and I. Martinson.

Physics Letters 97A, 187 (1983).

A CN^+ beam produced by stripping CN^- in the terminal of a

Pelletron tandem accelerator was dissociated in a thin carbon foil. Optical observation of ultraviolet transitions of C III, C IV and N IV, N V showed intensity variations as a function of foil thickness. The results indicate an enhancement of population due to the neighboring partner projectile for some but not all excited states.

GROUP 4. ANALYSIS OF SPECTRA FROM LASER-PRODUCED PLASMAS

Paper 8. The 3d-4f Transitions in S VII Observed in a Laser-Produced Plasma.

C. Jupén, U. Litzén and A. Trigueiros.

Physica Scripta 29, 317-318 (1984).

The energy levels of the $2p^5 4f$ configuration in Ne-like sulphur, S VII, have been derived from spectral lines in the region 330 - 375 Å. The lines, which were identified as belonging to the 3d-4f transition, were emitted from a laser-produced plasma. The structure in the 4f configuration has been studied through a parametric fit of Slater integrals.

3. THE EXPERIMENTAL FACILITIES FOR ATOMIC SPECTROSCOPY IN LUND

A) Beam-Foil Spectroscopy

The field of beam-foil spectroscopy was introduced by Kay [11] and Bashkin [12] in the early 1960's. It is now a standard method for studies of atomic spectra and lifetimes [13-19].

The method consists of accelerating ions and sending them through a carbon foil. The ions emerge from the foil in different stages of ionization and excitation. The light emitted from the decaying states can be spectroscopically investigated.

The set up of a beam-foil experiment is shown in fig. 1.

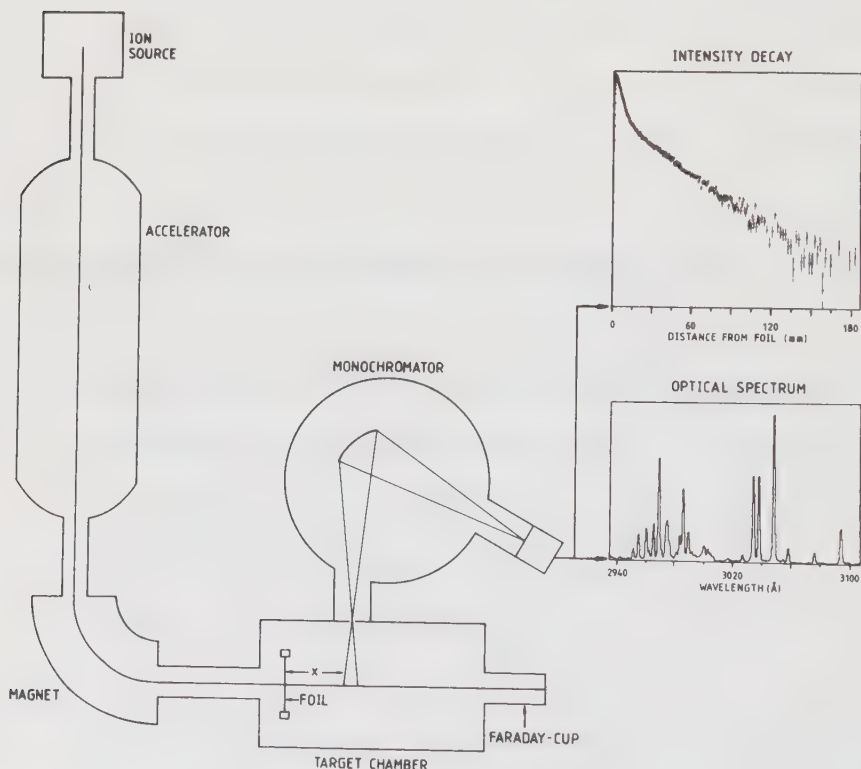


Fig. 1. The set up of the BF experiment in Lund [54].

a) The Pelletron accelerator

The facility used in our experiments is a Pelletron Tandem accelerator, model 3UDH, manufactured by the National Electrostatics Corporation (NEC), Wisconsin (USA). It was installed in the Physics Department at the University of Lund during 1975, and has been used for beam-foil experiments since 1977. The accelerator has a maximum terminal voltage of 3 MV and is equipped with a direct extraction duoplasmatron ion source.

The negative ion-beam is mass analysed by an inflection magnet and then enters the accelerator tube. In the high voltage terminal the negative ions pass a stripper gas region, where they lose several electrons through collisions with the gas molecules. The emerging positive ions are further accelerated to ground potential and then directed through a magnet, which is used both for energy analysis and for directing the ion-beam into the target chamber.

A diagram of the accelerator is shown in fig. 2. A detailed technical description of the accelerator can be found in [20].

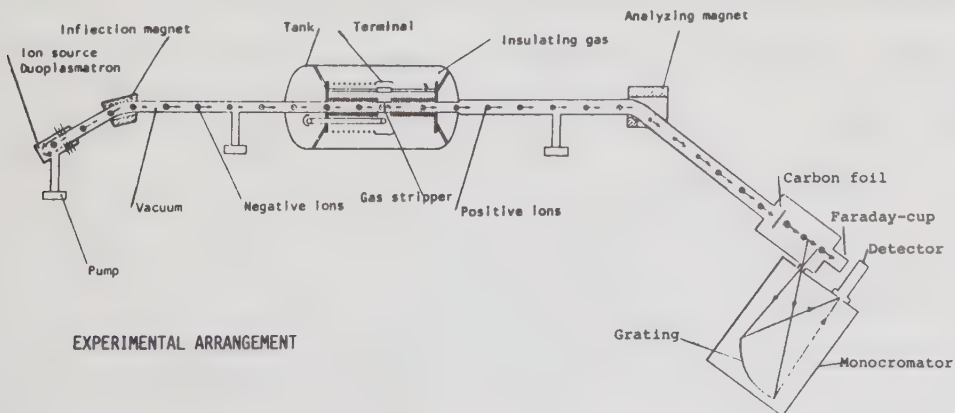


Fig. 2. A diagram of the Pelletron accelerator in Lund.

b) The beam-foil target chamber

After emerging from the analysing magnet, the ion beam enters the experimental beam line and the target chamber. The latter is made of aluminium sealed with O-rings. Its dimensions are 14x15x40 cm (approx) and the inner walls are covered with black paint in order to reduce reflected light. Approximately 20 carbon foils can be mounted on a wheel. The thickness of the foils is 2-20 $\mu\text{g}/\text{cm}^2$. The foil wheel is mounted on a carriage which can be translated parallel to the particle beam.

The translation of the foil wheel is done by means of a computer controlled stepping motor placed outside the chamber. A precision screw connects the stepping motor to the wheel via a high-vacuum feed-through. The pitch of the screw is 6 mm, giving a minimum displacement of 1/16 mm as the stepping motor moves 96 steps per revolution. The carriage can travel a distance of 232 mm between two end point switches. However, only 180 mm are available for lifetime measurements due to the position of the entrance slit.

After passing the carbon foil the ion-beam is collected by a Faraday cup.

c) Spectrograph detectors and data control

The spectrometer (monochromator) which has been used in our experiments is a Minuteman 1 m normal incidence vacuum spectrometer (310 NIV).

The detection technique used in our beam-foil experiments is photon counting. The detectors which have been used are: a Bendix CEM 4503 channel electron multiplier for wavelengths 300-1100Å, an EMR model 541F-08-18 photomultiplier tube for wavelengths 1050 - 2500 Å and an EMI model 9789 QB photomultiplier tube for wavelengths 1750-5500 Å.

The parts of the system for control of the experimental data are: a minicomputer, Alpha-LSI 2/20 with a 64 kB core memory, a Tektronix 4006 graphics terminal used for communication with the experiment, a Calcomp 565 digital plotter and a line-printer, model IDS-560 from Integral data Systems, Inc, for data presentation.

More details on the monochromator, the detection technique and the data control system can be found in Huldt's thesis [21] and in [22-24].

B) Laser Produced Plasmas

The spectroscopy of laser-produced plasmas is an important consequence of laser technology. The first laser, a ruby laser, was built in 1960 by Maiman [25]. However, laser-produced plasmas were possible only with the advent of the Q-switching technique in 1962 [26]. This technique permitted the generation of single light pulses with lengths of 10^{-8} s and peak powers of 10^9 W. Present high-power lasers, usually neodymium glass lasers operating at $1.06 \mu\text{m}$, can generate up to 2×10^{13} W focused to 10^{18} W/cm² in subnanosecond pulses [27].

Laser-produced plasmas are used in many different fields : 1) Fusion research, i.e., the compression of a plasma to high densities and pressures, to obtain a thermonuclear reaction with the eventual liberation of energy. Pressures of 4000 Mbar and densities of 10 g/cm^3 have been reached through laser-driven implosions of deuterium-tritium filled spherical-shell targets. The confined lifetime of these plasmas is less than 0.1 ns and their diameter is about $20 \mu\text{m}$. 2) Laser-produced plasmas are interesting as sources of electrons and highly stripped ions for use in particle accelerators. 3) Laser-produced plasmas are used as light sources in the analysis of spectra of highly ionised atoms [28-32]. The first experiment using the radiation from a plasma formed by a laser, was done by Ehler and Weisser in 1966 [33]. They used a 10 MW peak power ruby laser with a total energy of 0.4 J to produce a plasma with a temperature of the order of 10 eV. The experiment was done to determine the temperature of the plasma by measuring the wavelength at the peak intensity of the emitted continuum radiation.

a) High power laser for spectroscopy studies

The facility used to produce plasmas, by the Atomic Spectroscopy Group in Lund, is a Q-switched Neodymium -YAG/glass laser. The laser pulse length is 3 ns and the maximum energy obtained is 4.5 J. The laser power is thus about 1.5 GW.

The origin of the laser light is a flash lamp pumped Neodymium-doped YAG oscillator fig.3. The Q-switching device, consists of a $\lambda/4$ plate, a Pockels cell and a polarizer. After passing through a diaphragm (2), the light is deflected by a normal prism (3) and a Glan-Thompson prism (4). The pulse is then amplified by a second flash-lamp pumped Nd-YAG rod (5). After passing through a $\lambda/4$ plate (6) the light is reflected back (7) once more through the $\lambda/4$ plate and the Nd-YAG amplifier. The pulse now has the correct polarisation for transmission through the prism (4), after which it is bent around by the two mirrors (8) and (9). The laser pulse is then expanded and collimated by the two lenses (10) and (11), before being amplified for the last time. This last amplification is done by a flash lamp pumped Nd-Glass amplifier (12). The last element in the laser system is a Faraday rotator (13), which stops any externally reflected light from finding its way back into the laser system. This reflected light could otherwise be amplified by the laser rods and lead to damage to the system. Figure 3 shows a schematic description of the system above.

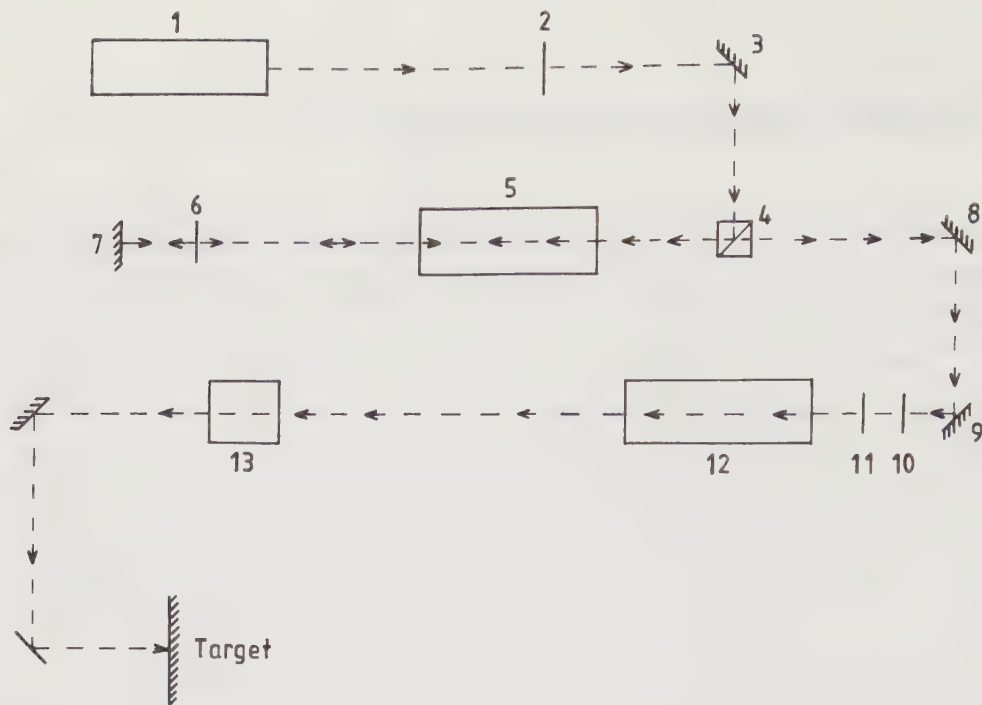


Fig.3. A schematic description of the Nd-YAG/glass Laser and its different parts.

b) The target chamber and the production of the plasma

After the last amplification the light is directed towards the target chamber, fig.4, using dielectric mirrors. The light from the laser is focused on to target by a lens with a focal length of 30 cm. Both lens and target can be moved to obtain the optimum power density and position of the plasma in front of the spectrograph slit.

The focusing of the radiation from the laser on the surface of the target (in vacuum) produces a plasma. Theoretical models have been developed to describe the plasma production and these differ depending upon whether the target is a conductor or an insulator [34].

In a conductor, the electromagnetic field of the laser radiation interacts strongly with the conduction electrons of the target. In the beginning of the laser pulse enough energy is thus transferred to the target to cause evaporation from the surface. Further absorption of radiation causes ionisation processes to occur. Through these processes a thin layer of dilute cold plasma is formed close to the target surface. In the case of a non-metallic target no free conduction electrons exist, and the initial plasma formation has to be described by more complex theories.

Once this initial plasma layer is formed, the energy during the later part of the laser pulse can be absorbed by the inverse bremsstrahlung process. The energy of the free electrons will therefore increase and lead to more ionisation. This process continues until the electron density is so high that the plasma reflects the incoming laser radiation, like a metal mirror. The increase in plasma temperature leads to an increase in the plasma volume (expansion), corresponding to an eventual decrease in the plasma density. A dynamic equilibrium is thus established [28]. Fig. 5 shows a sketch of the development of a laser-produced plasma and fig. 4 a schematic drawing of the target chamber: (A). Adjustment of lens relative to the target (focus). (B). Adjustment of lens and target relative to the optical axis of the spectrograph. (C). Stepmotor to rotate the target. (D). Adjustment of the target perpendicular to the incoming laser beam.

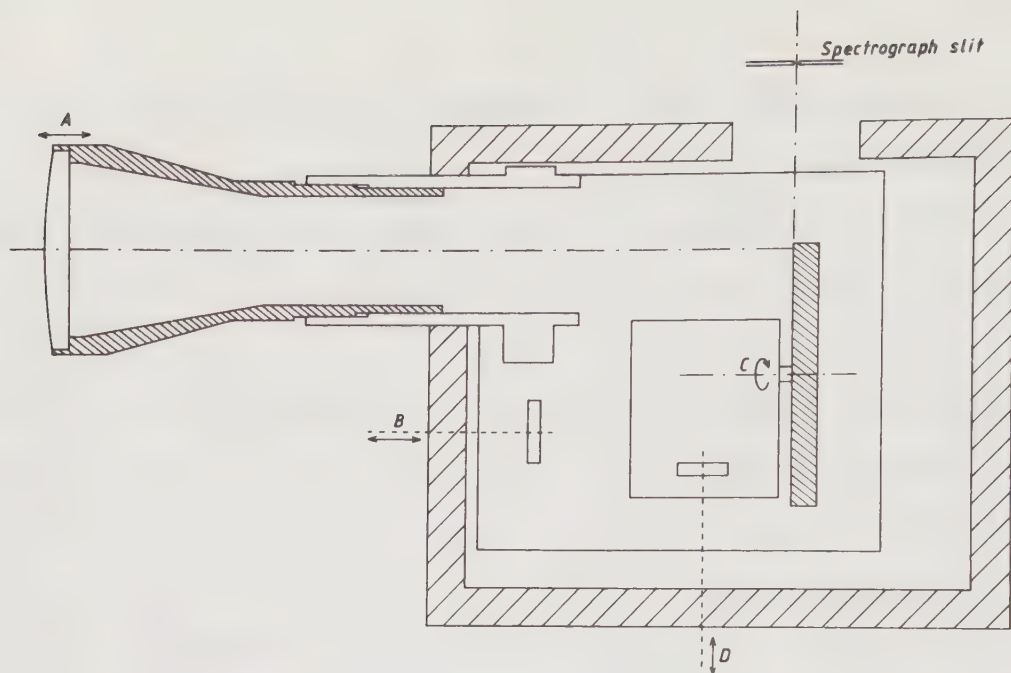


Fig. 4 A schematic drawing of the target chamber , (After Ekberg and Litzén [35]).

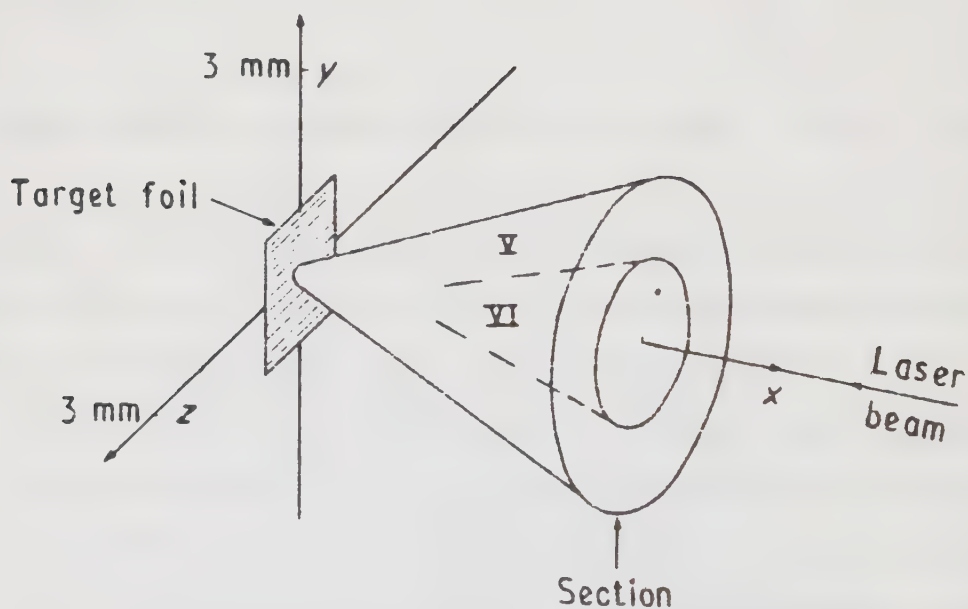


Fig. 5. An idealized picture of the spatial distribution of C V and C VI over the region $x=0-5$ mm at $t=45$ ns [34].

4. ANALYSES OF EXPERIMENTAL DATA

In this section we will describe the analysis of spectra obtained by the beam-foil method and also spectrum from laser-produced plasmas. In the next section, these results will be compared with calculations.

A) The Beam-Foil Method

As an example of the analysis we will consider our study of the spectrum of seven times ionised sulphur (S VIII) in the region 400-1100 Å. This deals with the transitions 3s-3p and 3p-3d, and the purpose is also to locate those 3p and 3d levels which do not combine with the ground state.

a) The necessary programs for wavelength determination

The wavelength spectra were first analysed by a program PEAKF described in appendix A of Huldt's thesis [21]. For blended line structures the positions were obtained by the program CARATE [53] which deconvolutes a sum of Gaussian shaped lines.

b) The charge distribution of the ions

To determine the ionisation degrees of the observed beam-foil lines, spectra were taken at different ion energies.

Figs. 7-8 show spectra (from 570 to 970 Å) of sulphur at 2 and 3 MeV. A comparison of the spectra shows that the lines of S V are more intense at 2 MeV than at 3 MeV, and the lines of S VIII are more intense in the spectrum at 3 MeV. It is well known that the higher ionisation stages become more dominant with increasing energy. Fig. 6 shows the distribution of sulphur ions in different degrees of ionisation as a function of ion energy.

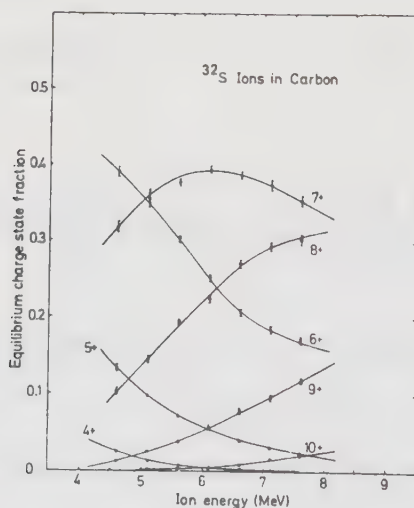


Fig. 6. The equilibrium charge state fractions for sulphur as a function of the beam energy, after Ambros and Kleinfeld [36].

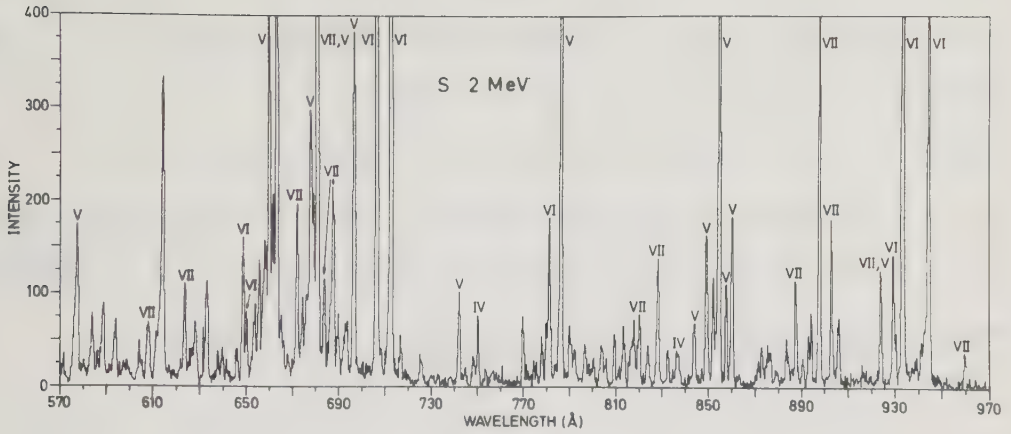


Fig. 7. The spectrum of sulphur at 2 MeV.

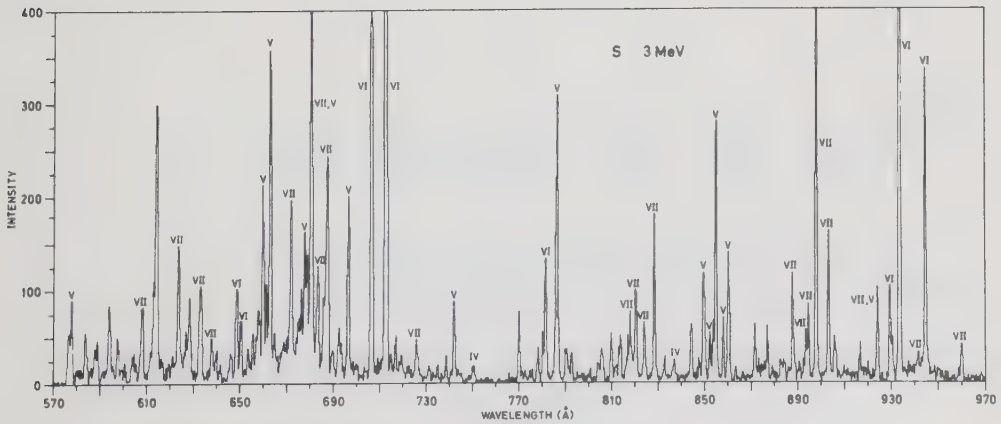


Fig. 8. The spectrum of sulphur at 3 MeV.

c) Isoelectronic extrapolation

In our case we have been interested in investigating the transitions $3s-3p$ and $3p-3d$ in seven times ionised sulphur (S VIII). Here a useful method is based on isoelectronic comparisons along the F I isoelectronic sequence [37]. As an example, fig. 9 shows an extrapolation of the transitions $3s\ ^4P_{5/2} - 3p\ ^4P_{5/2}$ along Na III, Mg IV, Al V and Si VI [40-43]. The value obtained from the extrapolation for S VIII is $959.70\ \text{\AA}$. The corresponding experimental value is $959.70\ \text{\AA}$. Thus, the extrapolated value agrees with the experimental one

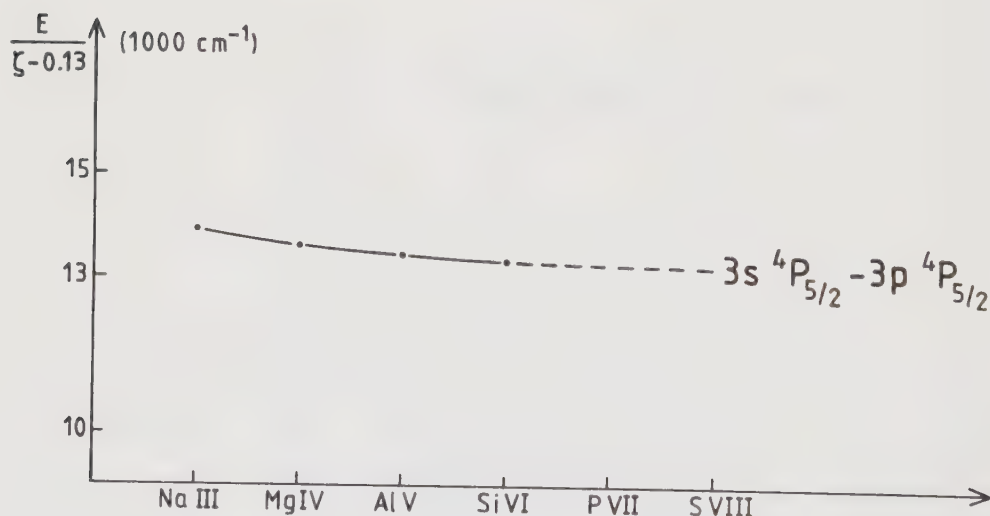


Fig. 9 The extrapolation of the transition $3s\ ^4P_{5/2} - 3p\ ^4P_{5/2}$ along Na III, Mg IV, Al V and Si VI. ζ = net charge of the core.

Now we can use the transition $3s\ ^4P_{5/2} - 3p\ ^4P_{5/2}$ as a base and extrapolate all the other transitions with reference to it. In fig.10 we see the extrapolation of $3s\ ^4P_{5/2} - 3p\ ^4D_{7/2}$ (849.76 Å) $3s\ ^4P_{3/2} - 3p\ ^4D_{5/2}$ (871.5 Å) and $3s\ ^4P_{1/2} - 3p\ ^4D_{1/2}$ (867.04 Å). The values from our experiment are 849.90 Å, 871.13 Å and 867.13 Å, respectively.

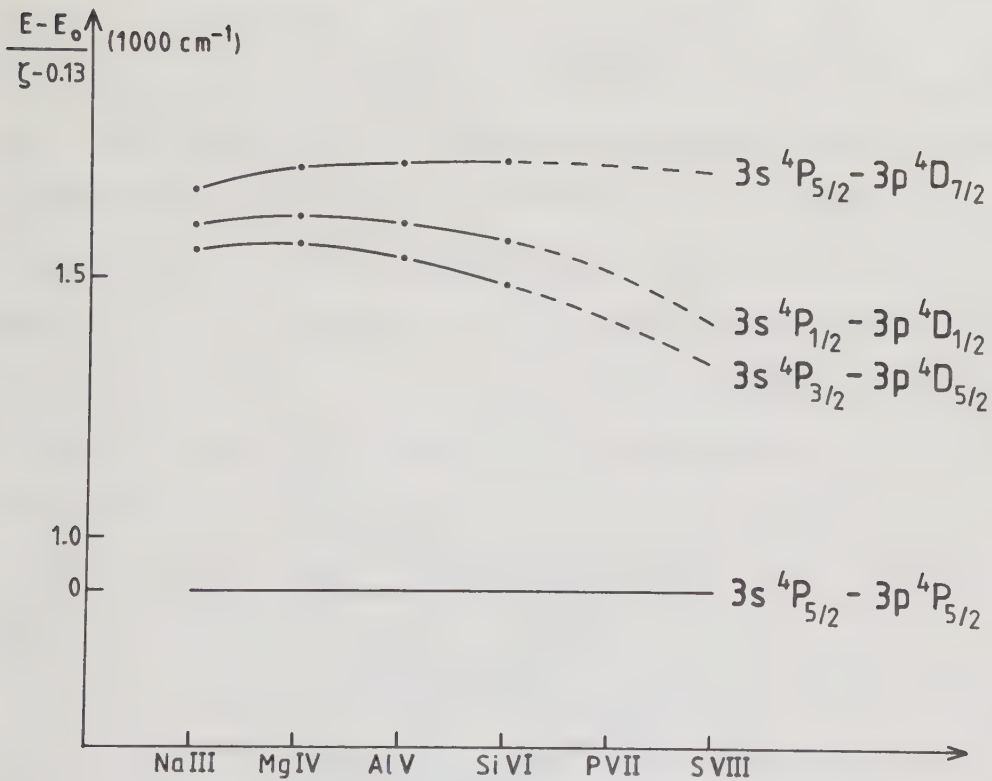


Fig. 10. A picture of some extrapolated transitions in S VIII.

Isoelectronic comparison for energy levels along F I isoelectronic sequence are shown in figs. 11 and 12.

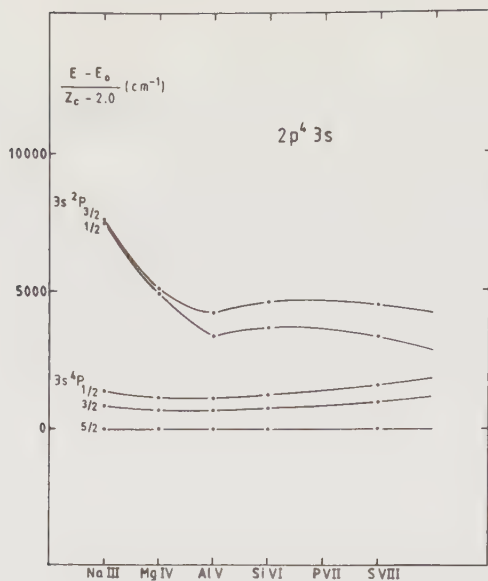


Fig. 11 Isoelectronic comparison for the $2p^4 ({}^3P) 3s$ levels.

$E_0 = E(3s {}^4P_{5/2})$, Z_c = net charge of the core and 2.0 is the value of an empirically adjusted constant.

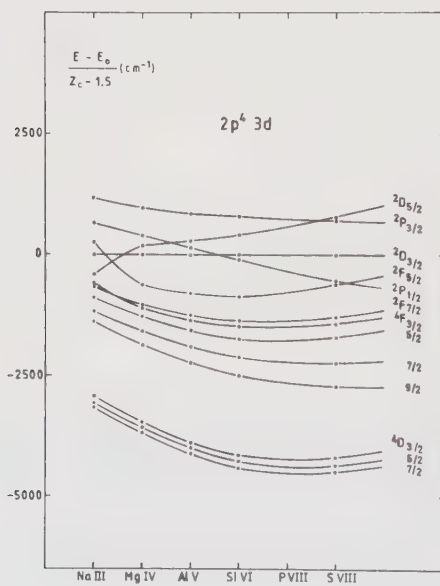


Fig. 12. Isoelectronic comparison for the $2p^4 ({}^3P) 3d$ levels (the term 4P is omitted). $E_0 = E(3d {}^2D_{3/2})$.

B) Laser Produced Plasmas

The spectra observed from a laser produced plasma can be understood from the simple model sketched earlier. The high electron density near the target surface gives rise to a continuous bremsstrahlung spectrum. Outside this area a line spectrum can be observed. If the spectrograph slit is parallel with the target surface short spectral lines are observed with a stigmatic photographic recording. At a greater distance from the target the observed lines are longer, corresponding to the conical expansion of the plasma, fig. 5 in this thesis. It is even possible to observe that higher ionisation stages give rise to shorter spectral lines, confirming that ions of higher ionisation stages move perpendicularly away from the target surface with higher velocities than the lower ionisation stages. This allows us the possibility of distinguishing between lines from different stages of ionisation.

Besides the analysis of the 3d-4f transitions in six times ionised sulphur, S VII, described in paper 8, work is also in progress on the 3d-4f transitions in seven times ionised sulphur, S VIII [38].

Work on 3d-4f transitions in the same isoelectronic sequence for Si VI is also planned [39].

5. Theoretical and Semi-empirical Treatment of the Spectra

The theory of the spectra is based on Quantum mechanics. Schrödinger's equation is the principal tool but this cannot be solved exactly for atoms with more than one electron. We therefore need to use approximation methods, such as the self-consistent-field method, first formulated by Hartree in 1928. The basic point in this approximation is the independent particle model or the central field approximation, according to which each electron moves in an effective potential, due to the attraction of the nucleus and the repulsive interactions between electrons. Each electron is described by its own wavefunction. Hartree wrote equations for the electron wavefunctions but these are not asymmetric in the electron coordinates. In 1930 Fock took into account the antisymmetric requirement for the wavefunctions. This generalization is known as the Hartree-Fock method.

The variational principle leads to Hartree-Fock equations [44-45]

Hartree-Fock Equations

$$\left[-\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} - \frac{2Z}{r} + \sum_{j=1}^q (w_j - \delta_{ij}) \int_0^\infty \frac{P_j^2(r_2) dr_2}{r_2^2} - (w_i - 1) A_i(r) \right] P_i(r) \\ = \epsilon_i P_i(r) + \sum_{j(\neq i)=1}^q w_j [\delta_{l_i l_j} \epsilon_{ij} + B_{ij}(r)] P_j(r)$$

The explanation of the different terms in the Hartree-Fock equations can be found in [44].

The Hartree-Fock equations can be solved by a program constructed by Froese Fischer [46]. This allow us to calculate wave functions, average energies, Slater integrals and spin-orbit parameters, for a single configuration. A WAVE-MANIP program [54] calculates configuration interaction integrals, multipole moments and plots the wave functions.

In seven times ionised sulphur (S VIII) we have calculated the necessary parameters for the configurations $2p^5$ (ground configuration), $2p^43s$, $2p^43p$ and $2p^43d$ (excited configurations).

The parameters we need are: total energy for the ground configuration, total energy for $3s$, $3p$ and $3d$ configurations, spin-orbit parameters, electrostatic parameters and the dipole moment. Below some tables with parameters calculated with the programs are given:

Table 1 Spin-Orbit Parameters and Average Energy (cm^{-1})

Configuration	E_{av}	ζ_{2p}	ζ_{3p}	ζ_{3d}
$2p^43s$	1588668	7110	-	-
$2p^43p$	1702885	7130	1127	-
$2p^43d$	1848153	7132	-	100

Table 2 Slater Integrals in (1000cm^{-1}) for the 3s configuration

$F^2(2p,2p)$	$G^1(2p,3s)$
231.990	18.820

Table 3 Slater Integrals in (1000cm^{-1}) for the 3p configuration

$F^2(2p,2p)$	$F^2(2p,3p)$	$G^0(2p,3p)$	$G^2(2p,3p)$
232.518	45.297	17.629	18.742

Table 4 Slater Integrals in (1000cm^{-1}) for the 3d configuration

$F^2(2p,2p)$	$F^2(2p,3d)$	$G^1(2p,3d)$	$G^3(2p,3d)$
232.008	50.876	40.830	23.342

The Wave-Manip program allows us to calculate the configuration interaction integrals (C.I.) integrals. This is important in our case because three configuration have the same parity, $2p^5$, $2p^43s$ and $2p^43d$. An application of the configuration interaction parameters is

found in paper 2, here we only give their values.

Table 5 C. I. Integrals for $2p^5$, 3s and 3d Configurations (in cm^{-1})

$R^1(2p2p, 2s3s)$	42594
$R^1(2p2p, 2s3d)$	-98464
$R^2(2p3s, 2p3d)$	24232
$R^1(2p3s, 3d2p)$	-5672

In table 5, the first integral takes into account the interaction between the configurations $2p^5$ and $2p^43s$, the second one includes the interaction between $2p^5$ and $2p^43d$ and the third and fourth take into account the interaction between 3s and 3d configurations.

In the analysis of atomic spectra much progress has been made by the introduction of effective parameters [47-52]. The introduction of the effective parameter $\alpha(2p, 2p)$ reduces the rms deviation of the configuration, but the other effective parameters are not important in the analysis of the 3s, 3p and 3d configurations. More details on these parameters can be found in paper 2 in this thesis.

The 3s wavefunction of the $2p^43s$ configuration in S VIII, is graphically presented in fig 13.

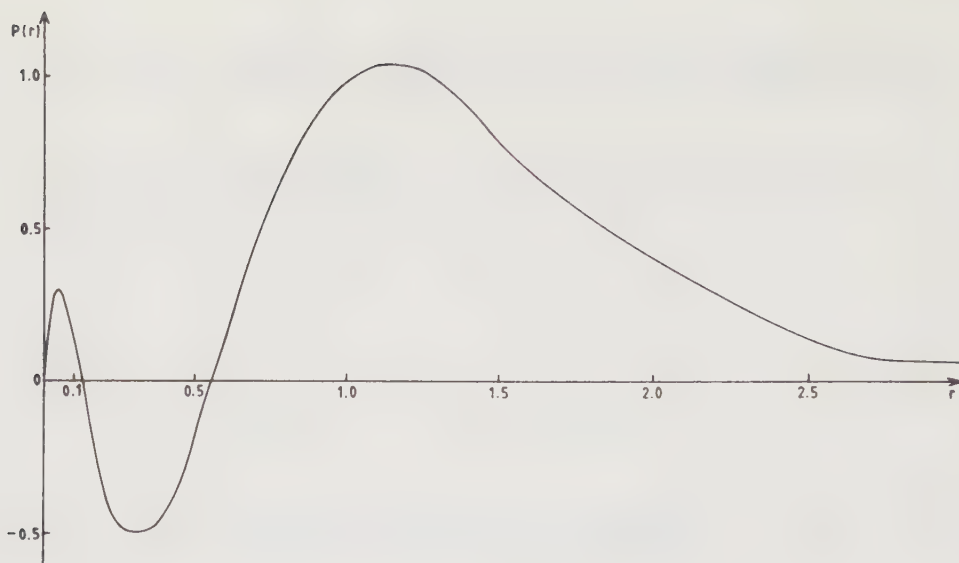


Fig. 13 A drawing of the 3s wavefunction in S VIII, using calculated values from the Hartree-Fock program.

The parameters calculated by the programs quoted above act as input values for two programs written by Cowan [55]. One program calculates eigenvectors, eigenvalues, transition probabilities and the purities in different couplings. The results can be found in paper 2.

Finally we can use a least-squares fitting program [55], also written by Cowan. The inputs for this program consist of the parameter coefficient matrices and transformation matrices calculated by the first Cowan program. The Hartree-Fock parameters and the experimental values of the energy levels also are part of the input to this program.

Calculations by the least-squares program give the fitted values for the Hartree-Fock parameters, the rms deviation to a configuration, the theoretical values for energy levels and the difference between experimental and calculated values for the energy levels. The results of the above calculations are given in paper 2.

6. RESULTS OF SPECTRAL ANALYSES AND LIFETIME MEASUREMENTS

In this section we present and comment on some results of spectral analyses and lifetime measurements.

A) Spectral Analyses

Information on the transitions $3s-3p$ and $3p-3d$ in S VIII, $3d-4f$ in S VII and energy levels for S VIII and S VII, was given in section 2 of this thesis. More detailed discussions on these spectra can be found in papers 1, 2 and 8. In this section (6a) we will confine ourselves to some comments on the transitions $1s2s2p^2 \ ^5P-1s2p^3 \ ^5S$ in F VI and the fine structure separations for the $1s2s2p^2 \ ^5P$ term in F VI. These transitions and fine structure separations are included in paper 3. For the transitions $1s2s2p \ ^4P-1s2p^2 \ ^4P$ and the fine structure separations for both 4P terms in F VII, detailed information can be found in paper 3.

A description of jK coupling for the $4f$ configuration, in six times ionised sulphur (S VII), is provided in section 6b.

a) Fine structure separations

The interest in the $1s2s2p^2 \ ^5P-1s2p^3 \ ^5S$ multiplet proceeds from the theoretical work of Bunge [56] which predicted that a line at 3489 Å, observed in many beam-foil studies of lithium [57-60] but not classified, was a transition between two multiply excited states in

the negative lithium ion, Li^- . This suggestion was verified, using the beam-foil method, by Mannervik et al [61], Brooks et al [62] and Denis and Desesquelles [63].

By beam-foil experiments the $1s2s2p^2\ ^5P$ fine structure has been resolved for C III [64], N IV [64], O V [64-65], F VI (paper 3 in this thesis) and Ne VII [66]. Here, considerable deviations from the Landé interval rule were noted, showing that not only is the effect of the spin-orbit interaction in the Hamiltonian necessary, but also the Breit operator which includes magnetic interaction and accounts for retardation effects, must be taken into account in the calculations, in order to reproduce the experimental data. Using the multiconfiguration Dirac-Fock optimal level (MCDF-OL) calculations, including the Breit interaction as a first order perturbation, Berry et al [64] calculated the transitions in the $1s2s2p^2\ ^5P-1s2p^3\ ^2S$ multiplet for ions in the Be I sequence up to $Z = 40$. The fine structure for C III, N IV, O V, F VI and Ne VII, calculated by the above MCDF-OL, shows good agreement with the beam-foil measurements, but the transition wavelengths show systematic differences from theory, see table 6. Later, Hata and Grant [67] performed calculations using a variation of the MCDF, MCDF-EAL (multi-configuration Dirac-Fock extended average level), on these ions. They improved agreement in the transition wavelengths, but for N IV and O V that have the best resolved fine structure measurements, the experimental values lay in between both calculations. Table 7, below gives experimental values for the fine structure splittings and a comparison with the calculations using the two different versions of MCDF, and fig. 14 shows the experimental and theoretical fine structure interval for $1s2s2p^2\ ^5P$ states.

Table 6. The mean transition wavelengths ($\text{\AA}$) for $1s2s2p^2\ ^5P-1s2p^3\ ^5S$
multiplet in F VI

Ion	Experiment	Theory[MCDF-OL] ^a	Theory[MCDF-EAL] ^b
C III	1016.06 $\pm$ 0.05a	989	1003.7
N IV	825.65 $\pm$ 0.05a	807	816.4
O V	694.75 $\pm$ 0.10a	682	688.1
F VI	599.67 $\pm$ 0.10 ^c	589 ^d	-
Ne VII	526.65 $\pm$ 0.10 ^e	520 ^d	-

a Berry et al [64].

b Hata and Grant [67].

c This thesis [paper 3].

d Cheng, Private communication in e

e Hardis et al [66].

Table 7. Fine structure splittings of $1s2s2p^2 \ ^5P$ (in cm^{-1})

Interval	Ion	Experiment	Theory[MCDF-OL] ^a	Theory[MCDF-EAL] ^b
J = 2-1	C III	63.5 ± 1.5^a	57	59.63
"	N IV	127.1^a	125	129.19
"	O V	252.4^a	242	247.34
"	F VI	453 ± 20^c	426	433.42
"	Ne VII	711 ± 22^d	700	708.25
J = 3-2	C III	-	21	30.16
"	N IV	79.5 ± 0.8^a	73	86.58
"	O V	188 ± 2^a	176	194.66
"	F VI	396 ± 20^c	354	378.50
"	Ne VII	680 ± 7^d	633	665.17

a Berry et al [64].

b Hata and Grant [67].

c This thesis [paper 3].

d Hardis et al [66].

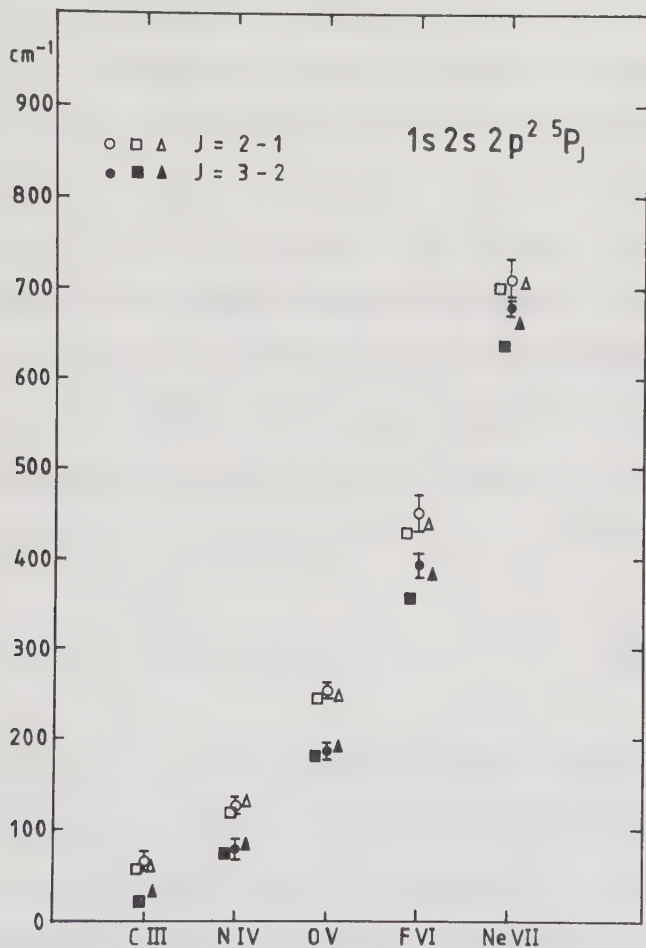


Fig. 14 Experimental and theoretical fine structure intervals of the $1s2s2p^2\ ^5P$ states. The circles are the experimental values. Boxes are the MCDF-OL calculations and the triangles are the MCDF-EAL calculations.

Conclusion: Wavelengths and fine structures of the transitions $1s2s2p^2 \ ^5P-1s2p^3 \ ^5S$ in C III, N IV, O V, F VI and Ne VII, have been compared to theoretical values obtained using two versions of the multi-configuration Dirac-Fock calculations (MCDF-OL and MCDF-EAL). Theory does not quite reproduce the experimental wavelengths while agreement for the fine structure is satisfactory. The theoretical values have been calculated as in [94]. Refinements in calculating the retardation term in the Breit may lead to even better agreement. For the Li I sequence Chen et al [95] have calculated both quartet terms accurately and obtained good agreement with the experimental fine structure for $1s2s2p \ ^2P$ and $1s2p^2 \ ^4P$ terms. More recently, the $1s2s2p \ ^4P-1s2p^2 \ ^4P$ multiplet has also been investigated for Ne VIII, using the beam-foil technique [68]. Accurate calculations, besides those mentioned in paper 3 have also been reported by Hata and Grant [69] and Chung [70].

b) jK-coupling

In the analysis of the $3d-4f$ transition in six times ionised sulphur S VII, [paper 8], observed in a laser-produced plasma, the $2p^54f$ configuration is described by pair coupling. The fundamental characteristic in this kind of coupling is that the energy levels tend to appear in pairs. This structure was first observed by Shenstone [71]. One form of pair coupling is jK-coupling, sometimes also called j1-coupling [72]. In excited configurations in which the excited electrons have large angular momenta and tend not to penetrate the core, the jK-coupling scheme gives a good description of the level structure. In our example, in paper 8, the core is formed by $2p^5$

electrons and the excited electron is 4f. The angular momentum coupling scheme for $2p^5[{}^2P]4f$ is:

1) J_c Total angular momentum for the core $2p^5$ [$J_c = 3/2, 1/2$]

2) $J_c + l_2 = K$ [$l_2 = 3$ for the f electron].

[$K = 9/2, 7/2, 5/2, 3/2$ for $J_c = 3/2$ and $K = 7/2, 5/2$ for $J_c = 1/2$]

3) $K + s_2 = J$ [$s_2 = \text{spin of the f electron}$]

[$J = 5, 4$ for $K = 9/2$; $J = 4, 3$ for $K = 7/2$; $J = 3, 2$ for $K = 5/2$ and $J = 2, 1$ for $K = 3/2$]

or $\{[(1, s, \dots) J_c, l_2] K, s_2\} J$

and for the energy level notation

$J_c [K] J$

If the excited electron does not penetrate the core, the development of the energy level structure in the jK-coupling is, for $2p^5({}^2P)4f$:

1) The strongest interaction is the spin-orbit interaction of the p electron in the core, producing the major energy separation for the two possible values of J_c (3/2, 1/2).

2) The next strongest interaction is the spin-independent (direct) part of the Coulomb interaction between the electrons of the core ($2p^5$) and the excited electron ($4f$). The separation of the energy levels goes according to the values of K .

3) Finally, the small spin-dependent (exchange) Coulomb interaction for the $4f$ electron and the small spin-orbit interaction of the $4f$ electron, produces a splitting into level pairs according to the two values of $J = K \pm 3/2$ and $J = K \pm 1/2$.

Table 8 shows the energy levels of the $4f$ configuration in S VII. The designations are given in an abbreviated jK-notation. The complete designation for the first level in the table should read $2p^5(^2P_{3/2})4f[9/2]_5$. In table 9 the energy for $K = 9/2$ is split in two levels $J=5$ and $J=4$. The separation between them is only 69cm^{-1} . Such a splitting of the energy levels in pairs with a small difference between them is a characteristic of jK-coupling. Fig. 14 illustrates the jK-coupling for the energy levels from table 9.

Table 9. Energy levels of $2p^54f$ in S VII

Designation	J	Energy (cm^{-1})
$(3/2)[9/2]$	5	1928503

	4	1928572
$(3/2)[7/2]$	4	1929745
	3	1929698
$(3/2)[5/2]$	3	1928804
	2	1929017
$(3/2)[3/2]$	2	1927682
	1	1927537
$(1/2)[7/2]$	4	1939112
	3	1939064
$(1/2)[5/2]$	3	1938964
	2	1939101

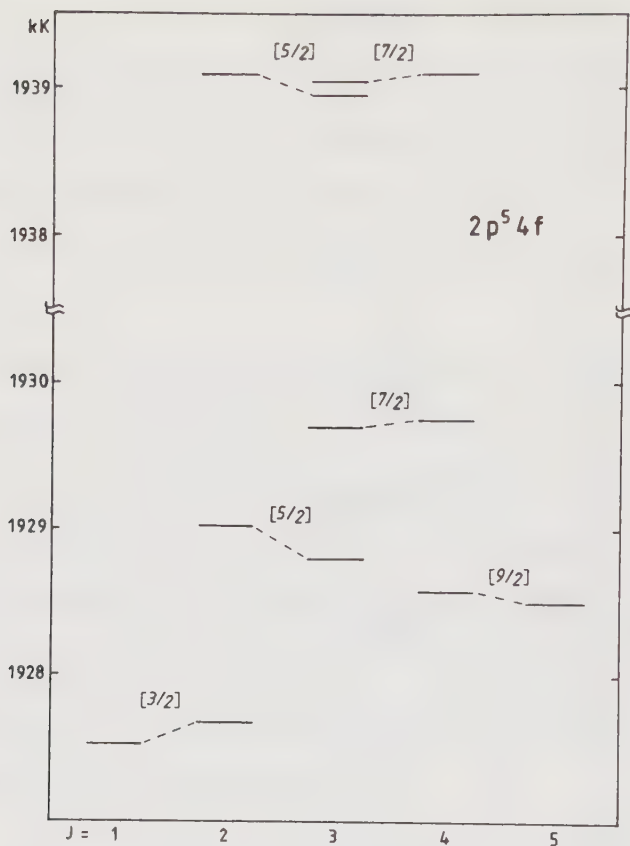


Fig. 14. Energy levels of the $2p^5 4f$ configuration in S VII.

The experimental data shows that jK -coupling describes the levels of the $2p^5 4f$ configuration. It is, however, not an extreme case of jK -coupling, as can be seen from the Slater integrals. In fact $F^2(2p, 4f)$ has approximately the same size as ζ_{2p} [44].

B) Lifetime Measurements by the Beam-Foil Method

The beam-foil technique is the only method for measuring lifetimes in highly ionised atoms. Lifetimes measurable by the beam-foil method lie in the range from 10^{-6} to 10^{-12} s.

The beam-foil technique for measuring lifetimes of excited levels has been described in many books and theses. A good description of this method is found in Curtis [73] who together with Berry and Bromander introduced the ANDC method to analyse decay curves with cascades. Recently Engström in his thesis [54] gave a review of new results of beam-foil lifetime measurements. There we can also find a description of the programs, LIFE, DECFIT, DISCPREP, DISCRETE and CANDY, used to analyse decay curves from beam-foil measurements.

Here I will give a systematic overview of the transition $2s^2\ ^1S - 2s2p\ ^1P$ in Be I -like ions from Be I to O V.

Experimental and theoretical f -values for the $2s^2\ ^1S - 2s2p\ ^1P$ transition in this sequence show some discrepancies in the interval B II - Ne VII [74]. In Be I there is an excellent agreement between the beam-foil result of Martinson et al. [75] and the theoretical data, but from B II on the experimental values have disagreed with theory. It has been suggested that the reason for this disagreement is incomplete correction for cascades in the beam-foil decay curves. In particular the $2p^2\ ^1S$ level which populates the $2s2p\ ^1P$ term, and which has a short lifetime, may cause difficulties. In paper 4 we measured the decays of $2p^2\ ^1S$ and $2p^2\ ^1D$ levels and these data were incorporated into the analysis of the $2s2p\ ^1P$ decay curve in N IV and O V.

The f -values for Be I-like ions are of great importance for astrophysical [76] and laboratory plasmas [77]. We show below a table with the experimental and theoretical data for f -values in the Be I sequence, for the $2s^2 \ ^1S$ - $2s2p \ ^1P$ transition. A figure of f as a function of $1/Z$ is also given.

Table 7.	Oscillator strength (f)		Wavelength (λ)
	Exp.	Theory ^a	(in Å)
Be I	$1.34 + 0.05^b$	1.40	2348.60
B II	$0.98 + 0.08^c$	1.03	1362.00
C III	$0.65 + 0.03^d$	0.80	977.00
N IV	$0.62 + 0.02^e$	0.61	765.15
O V	$0.53 + 0.02^e$	0.52	629.73

a) Hibbert [78]

b) Martinson, Gaupp and Curtis [75]

c) S. Bashkin, L.C. McIntyre, H.V. Buttler, J.O. Ekberg and
I. Martinson, to be published.

d) Heroux, Buchet-Poulizac and Buchet [79-80]

e) Engström, Denne, Ekberg, Jones, Jupén, Litzén, W.T.Meng, Trigueiros and Martinson (paper 5).

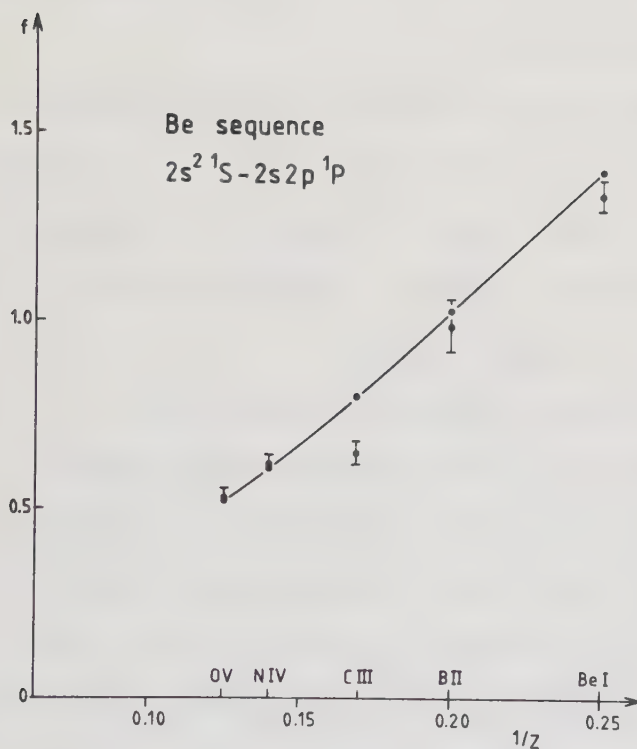


Fig. 15. f -value vs. $1/Z$ for $2s^2\ ^1S - 2s2p\ ^1P$ transition of the beryllium sequence.

Conclusion: Lifetime measurements and oscillator strengths are reported for the $2s2p\ ^1P$ level in Be-like N IV and O V. A study, for the same level, in Be I, B II and C III and comparison with theoretical values is made. The experimental results are in agreement with

theory. The discrepancy between theory and experiment in this sequence is removed when the most prominent cascades that repopulate the $2s2p\ ^1P$ level are explicitly included in the analysis made by the ANDC method. However, a new experimental measurement, using the beam-foil technique and introducing the above method for the analysis of the decay curves may be necessary for C III, because its experimental f -value disagrees with theory.

Two papers in this thesis deal with lifetimes in the Na I sequence. Even here, the theoretical and experimental f -values disagreed in several cases. The reason for the disagreement (as in the Be I sequence) is largely incomplete correction for cascades in the analyses of the decay curves.

In the analysis of the $3p\ ^2P$ decay curves in five times ionised sulphur(S VI) by the ANDC method, cascading from $3d\ ^2D$, $4d\ ^2D$ and $4s\ ^2S$ was included. The three cascades contain information on additional cascading from higher terms. The inclusion of the $3p\ ^2P$ - $3d\ ^2D$ decay curve in the analysis reduced the $3p\ ^2P$ lifetime from 0.74 ns to 0.63 ns. Cascading from $4d\ ^2D$ further reduced the $3p\ ^2P$ lifetime to 0.58-0.60 ns. The $4s\ ^2S$ cascading seemed to have no substantial effect. In Cl VII, unfortunately, we had to include fewer cascading because the $3p\ ^2P$ - $4s\ ^2S$ multiplet at 294 Å lies outside the detection range of our monochromator. However, as noted, this cascade had no substantial effect in S VI and our Cl VII data are therefore estimated to be as accurate as the S VI results.

Table 8 shows f -values (experiment and theory) for Na I-like ions from Na I to Cl VII, and fig.15 shows a comparison between theoretical and experimental f -values in the Na I sequence.

Table 8. Oscillator strength (f) Wavelength (λ)

 Exp. theory^a: (in Å)

Na I	0.954+0.0016 ^b	0.947	5892
Mg II	0.880+0.07 ^c	0.899	2796
Al III	0.770+0.03 ^d	0.831	1855
Si IV	0.73 +0.24 ^e	0.766	1397
P V	0.70 +0.15 ^f	0.707	1121
S VI	0.66 +0.02 ^g	0.658	937.1
Cl VII	0.603+0.015 ^h	0.614	804.8

a) Lindgård and Nielsen [81].

b) Gaupp, Kuske and Andrä [82].

c) Lundin, Engman, Hilke and Martinson [83].

d) Kernahan, Pinnington, O'Neill , Brooks and Donnelly [84].

- e) Berry, Bromander, Curtis and Buchta [85].
- f) Curtis, Martinson and Buchta [86].
- g) Ekberg, Engström, Bashkin, Denne, Huldt, Johansson, Jupén, Litzén, Trigueiros and Martinson (paper 5).
- h) Jupén, Engström, Huldt, Trigueiros, Ekberg, Litzén and Martinson (paper 6).

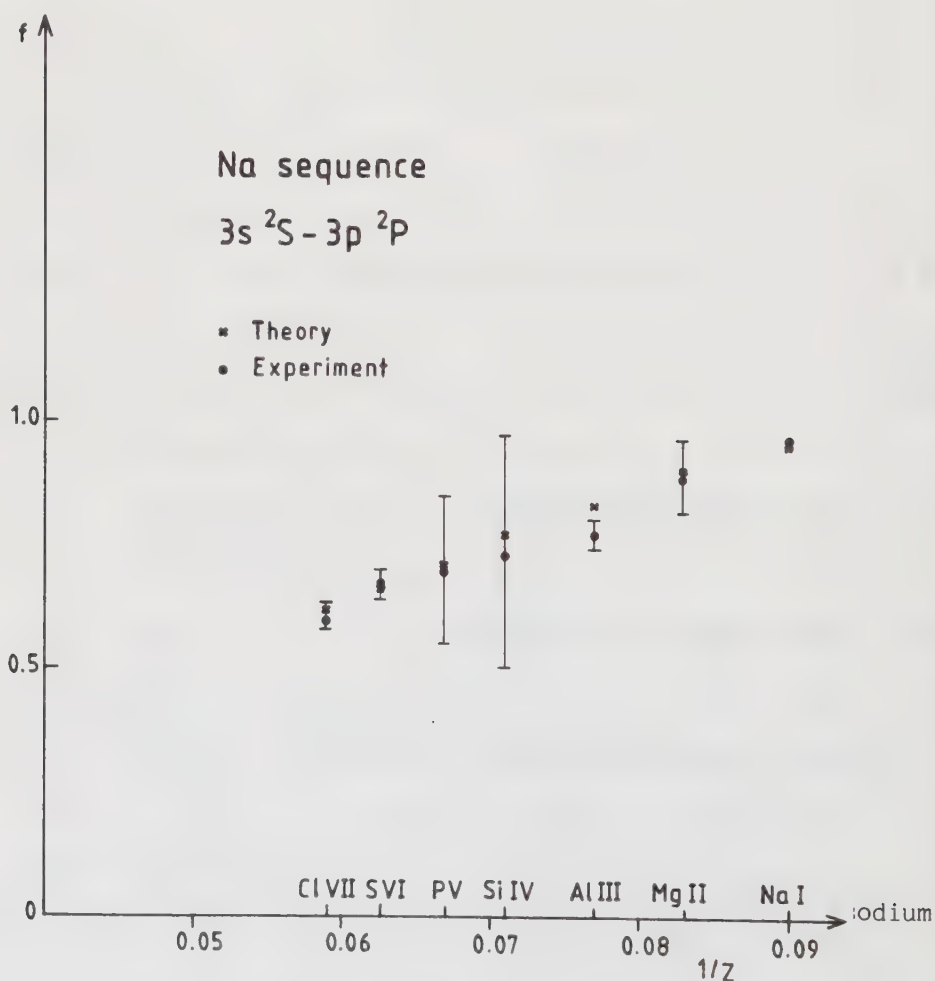


Fig.16. f -values vs. $1/Z$ for $3s\ ^2S - 3p\ ^2P$ transition in the sodium sequence.

Conclusion: We have measured the lifetimes and oscillator strengths for the $3s\ ^2S-3p^2P$ multiplet in S VI and Cl VII. Our results, taking into account the most prominent cascading by means of the ANDC method, are in good agreement with the theoretical calculation done by Lindgård and Nielsen [81] using a numerical Coulomb approximation program. We may conclude that most theoretical calculations of f -values are reliable in the case of the Na I sequence. A number of such theoretical references is given in papers 5 and 6 of this thesis.

6. Dissociation of Fast Molecular Ions into Atomic Excited States

The foil dissociation of fast molecular ions and the spectral analysis of the fragments resulting from this dissociation, give some interesting information on plasma oscillations in solids, stereochemical structures of molecular ions and collision processes [87-88].

The interaction processes of the molecular ions with the carbon foil are very complicated, but some information is available on these process [89-93].

In paper number 7 we have a CN^+ molecular beam produced in our tandem accelerator. The CN^- molecular ion beam is produced in a duoplasmatron ion source, accelerated and stripped in the terminal and finally we obtained about 100 nA CN^+ molecular ion beam in the chamber. When this beam passes through the carbon foil, the molecules break up in various C and N atomic ions and the light emitted downstream of the foil, emanating from C and N excited states, is spectroscopically analysed. More details on the experiment and the

results obtained can be found in paper 7. Other experiments are planned using molecular ions the aim being to obtain more quantitative data than those given in paper 7.

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